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=> index chemistry bioscience
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FILE 'DRUGMONOG' ACCESS NOT AUTHORIZED
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                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

INDEX 'AGRICOLA, ALUMINIUM, ANABSTR, APOLLIT, AQUALINE, AQUIRE, BABS, BIOTECHNO,
       CABA, CAOLD, CAPLUS, CBNB, CEABA-VTB, CERAB, CIN, COMPENDEX, CONFSCI,
       COPPERLIT, CORROSION, DISSABS, ENCOMPLIT, GENBANK, INSPEC, INSPHYS, IPA,
       KOSMET, METADEX, NAPRALERT, ...' ENTERED AT 23:27:31 ON 09 OCT 2007

92 FILES IN THE FILE LIST IN STNINDEX

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search error messages that display as 0* with SET DETAIL OFF.

=> s (peptide amphiphil?) (P) (nanofiber? or nanostructure? or nanotube? or
nanoparticle? or nanocluster? ) (P) metal?
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          0*  FILE APOLLIT
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          0*  FILE CAOLD
          2   FILE CAPLUS
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          0*  FILE CEABA-VTB
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          1*  FILE INSPEC
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          0*  FILE KOSMET
          1*  FILE METADEX
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          0*  FILE RAPRA
          1   FILE SCISEARCH
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          0*  FILE FOMAD
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          0*  FILE FROSTI
          0*  FILE FSTA
          3   FILE IFIPAT
          1   FILE LIFESCI
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          0*  FILE PHARMAML
  84 FILES SEARCHED...
          5   FILE USPATFULL
          1   FILE WPIDS
          1   FILE WPINDEX

  17 FILES HAVE ONE OR MORE ANSWERS,   92 FILES SEARCHED IN STNINDEX

L1   QUE (PEPTIDE AMPHIPHIL?) (P) (NANOFIBER? OR NANOSTRUCTURE? OR NANOTUBE? OR
       NANOPARTICLE? OR NANOCLUSTER? ) (P) METAL?

=> D rank
F1            5   USPATFULL
F2            3   IFIPAT
F3            2   CAPLUS
F4            2   DISSABS
F5            2*  PASCAL
F6            1   SCISEARCH
F7            1   EMBASE
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F9            1   MEDLINE
F10           1   WPIDS
F11           1   WPINDEX
F12           1*  INSPEC
F13           1*  METADEX
F14           1*  ANTE
F15           1*  BIOTECHABS
F16           1*  BIOTECHDS
F17           1*  ESBIOBASE


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COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                5.04       5.25

FILE 'IFIPAT' ENTERED AT 23:32:06 ON 09 OCT 2007
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FILE 'WPINDEX' ACCESS NOT AUTHORIZED

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L3 2 FILE CAPLUS
L4 2 FILE DISSABS
L5 1 FILE SCISEARCH
L6 1 FILE EMBASE
L7 1 FILE LIFESCI
L8 1 FILE MEDLINE
L9 1 FILE WPIDS

TOTAL FOR ALL FILES
L10 12 L1

=> dup rem L10
PROCESSING COMPLETED FOR L10
L11 10 DUP REM L10 (2 DUPLICATES REMOVED)

=> d l11 1-10 ibib abs

L11 ANSWER 1 OF 10 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 2007:381974 SCISEARCH
THE GENUINE ARTICLE: 149HT
TITLE: Perspectives on main-chain hydrogen bonded supramolecular polymers
AUTHOR: Shimizu, Linda S. (Reprint)
CORPORATE SOURCE: Univ S Carolina, Dept Biochem & Chem, Columbia, SC 29208 USA (Reprint)
shimizul@mail.chem.sc.edu
COUNTRY OF AUTHOR: USA
SOURCE: POLYMER INTERNATIONAL, (APR 2007) Vol. 56, No. 4, pp. 444-452.
ISSN: 0959-8103.
PUBLISHER: JOHN WILEY & SONS LTD, THE ATRIUM, SOUTHERN GATE, CHICHESTER PO19 8SQ, W SUSSEX, ENGLAND.
DOCUMENT TYPE: General Review; Journal
LANGUAGE: English
REFERENCE COUNT: 119
ENTRY DATE: Entered STN: 12 Apr 2007
Last Updated on STN: 12 Apr 2007
*ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS*

AB Supramolecular polymers are assembled from monomeric units held together by reversible non-covalent interactions. These supramolecular materials display polymeric properties and may soon have important industrial applications. This mini review focuses on the advances in main-chain supramolecular polymers whose assembly is guided primarily by hydrogen bonding interactions. The design constraints of these new systems discussed include assembly motifs, the strength and directionality of the non-covalent interactions, association versus reversibility, and environmental effects on the degree of polymerization. Selected literature examples including Meijer's ureidopyrimidinone system are used to highlight the challenges and potential of these supramolecular polymeric materials. (C) 2007 Society of Chemical Industry.

L11 ANSWER 2 OF 10 DISSABS COPYRIGHT (C) 2007 ProQuest Information and Learning Company; All Rights Reserved on STN
ACCESSION NUMBER: 2007:35669 DISSABS Order Number: AAI3237006
TITLE: Carbon nanotubes: Photophysics, biofunctionalization, and sorting via density differentiation
AUTHOR: Arnold, Michael Scott [Ph.D.]; Stupp, Samuel I. [advisor]; Hersam, Mark C. [advisor]
CORPORATE SOURCE: Northwestern University (0163)

SOURCE: Dissertation Abstracts International, (2006) Vol. 67, No. 10B, p. 5994. Order No.: AAI3237006. 305 pages. ISBN: 978-0-542-90858-3.
DOCUMENT TYPE: Dissertation
FILE SEGMENT: DAI
LANGUAGE: English
ENTRY DATE: Entered STN: 20070702
Last Updated on STN: 20070702

AB Carbon nanotubes, discovered in 1991, are relatively new materials with outstanding properties that make them attractive for applications in electronics, optics, high strength composites, and sensing. This thesis details new discoveries in the study of the photophysical properties of single-walled carbon nanotubes (SWNTs), the biofunctionalization of their surfaces using peptide amphiphiles, and their separation by physical and electronic structure.

To gain insight into the photophysical properties of these one-dimensional materials, a series of optical studies on isolated, surfactant-encapsulated SWNTs were explored. Specifically, transient photobleaching in semiconducting SWNTs was probed in response to optical excitation. It was observed that photobleaching quenched at acidic pH, was maximized for collinear polarization of pump and probe beams, and saturated with increasing pump and probe intensities. In time resolved measurements, the transient photobleaching was observed to decay on the order of 10-100 ps.

Additionally, the biofunctionalization of carbon nanotubes has been demonstrated by using peptide amphiphiles each consisting of a short hydrophobic alkyl tail coupled to a more hydrophilic, variable, bioactive peptide sequence. The functionalization was characterized using transmission electron microscopy, and sharp excitonic optical transitions were observed by absorbance spectroscopy confirming the debundling of aggregated SWNTs. Preliminary experiments in which neonatal rat cardiomyocytes were cultured on top of percolating networks of nanotubes suggest that they can be used as viable, electronically active substrates for in vitro cell culture.

Finally, a technique for the bulk enrichment and separation of SWNTs by diameter and band gap or by electronic type (metallic versus semiconducting) through ultracentrifugation in aqueous density gradients has been developed. Methods for sorting SWNTs by their physical and electronic structures are essential for future electronic and optical applications where mono-disperse SWNTs are needed. The mode and quality of separation via density gradient ultracentrifugation can be engineered by varying the nature of the encapsulating molecules utilized. For example, separation by diameter and band gap is readily achieved using oligomers of single-stranded DNA or bile salts. Furthermore, by tuning the structure-density relationship for SWNTs and their associated encapsulating molecules through addition of co-surfactants, separation by electronic type is possible.

L11 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:270780 CAPLUS
DOCUMENT NUMBER: 146:184710
TITLE: Intermolecular forces in the self-assembly of peptide amphiphile nanofibers
AUTHOR(S): Stendahl, John C.; Rao, Mukti S.; Guler, Mustafa O.; Stupp, Samuel I.
CORPORATE SOURCE: Departments of Materials Science and Engineering, Chemistry Feinberg School of Medicine, Northwestern University, Evanston, IL, 60208-3108, USA
SOURCE: Advanced Functional Materials (2006), 16(4), 499-508
CODEN: AFMDC6; ISSN: 1616-301X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Peptide amphiphile mols. (PAs) developed in our laboratory self-assemble from aqueous media into three-dimensional networks of bioactive nanofibers. Multiple non-covalent interactions promote assembly of the supramol. nanofibers and ultimately determine the bulk phys. properties of the macroscopic gels. In this study, we use oscillatory rheol., Fourier-transform IR spectroscopy, and circular-dichroism spectroscopy to better understand the assembly mechanism of a typical PA mol. known as PA-1. Self-assembly of PA-1 is triggered by counterion screening and stabilized by van der Waals and hydrophobic forces, ionic bridging, and coordination and hydrogen bonding. The concentration, electronic structure, and hydration of counterions significantly influence self-assembly and gel mech. properties.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:248986 CAPLUS
TITLE: Self-assembled enzyme mimic nanostructures
AUTHOR(S): Guler, Mustafa O.; Stupp, Samuel I.
CORPORATE SOURCE: Department of Chemistry, Northwestern University, Evanston, IL, 60208, USA
SOURCE: Abstracts of Papers, 231st ACS National Meeting, Atlanta, GA, United States, March 26-30, 2006 (2006), ORGN-271. American Chemical Society: Washington, D. C.
CODEN: 69HYEC
DOCUMENT TYPE: Conference; Meeting Abstract; (computer optical disk)
LANGUAGE: English

AB Self-assembling peptide amphiphiles (PAs) were designed to form high-aspect-ratio nanofibers that can present functional groups in high d. on their periphery. Nanofiber formation was confirmed by transmission electron microscopy (TEM). We incorporated sites that could catalyze ester hydrolysis at the termini of these self-assembling mols. so they could be displayed upon self-assembly on the surface of the nanostructures they form. The reactive sites were designed with histidine residues or with a metal coordinating groups for the hydrolysis of 2, 4-dinitrophenyl acetate (DNPA) or 2-hydroxypropyl p-nitrophenyl phosphate (HPNP). Pseudo-first order rates of ester hydrolysis in the presence of the nanofibers was studied by UV-Vis spectroscopy and calculated using the Michaelis-Menten reaction kinetics model. Faster hydrolysis rates were observed in the self-assembled system than in solution, likely due to the high d. of reactive sites on the surface of these fiber-shaped nanostructures. This concept could be extended to other enzyme mimics through presentation of appropriate amino acid residues on nanofiber surfaces.

L11 ANSWER 5 OF 10 IFIPAT COPYRIGHT 2007 IFI on STN

AN 04237351 IFIPAT;IFIUDB;IFICDB
TITLE: ENCAPSULATION OF NANOTUBES VIA SELF-ASSEMBLED NANOSTRUCTURES; FOR USE IN SYNTHESIS OF CARBON FIBERS
INVENTOR(S): Arnold; Michael Scott, Evanston, IL, US
Messsmore; Benjamin W., Evanston, IL, US
Stupp; Samuel I., Chicago, IL, US
Zubarev; Eugene RT., Ames, IA, US
PATENT ASSIGNEE(S): Northwestern University, Evanston, IL, US
PRIMARY EXAMINER: Le, H Thi
AGENT: Miller, Raymond
Pepper Humilton LLP

| | NUMBER | PK | DATE |
|---|---|---|---|
| PATENT INFORMATION: | US 6890654 | B2 | 20050510 |
| | (CITED IN 001 LATER PATENTS) | | |

US 2004022718 A1 20040205
APPLICATION INFORMATION: US 2003-418474 20030418
EXPIRATION DATE: 18 Apr 2023

| | NUMBER | DATE |
|---|---|---|
| PRIORITY APPLN. INFO.: | US 2002-373827P | 20020418 (Provisional) |
| FAMILY INFORMATION: | US 6890654 | 20050510 |
| | US 2004022718 | 20040205 |

DOCUMENT TYPE: Utility
Granted Patent - Utility, with Pre-Grant Publication
FILE SEGMENT: CHEMICAL
GRANTED
ENTRY DATE: Entered STN: 11 May 2005
Last Updated on STN: 6 Feb 2006

GOVERNMENT INTEREST:

The United States Government may have certain rights to this invention pursuant to work funded thereby at Northwestern University under grants from the National Science Foundation Grant No. EEC-0118025 W Main N602.

PARENT CASE DATA:

This application claims priority from U.S. Provisional Application Ser. No. 60/373,827 filed Apr. 18, 2002 the contents of which are incorporated herein by reference in their entirety.

NOTE: INDEXED FROM APPLICATION
Subject to any Disclaimer, the term of this patent is extended or adjusted under 35 USC 154(b) by 161 days.
MICROFILM REEL NO: 014551 FRAME NO: 0458
NUMBER OF CLAIMS: 28
GRAPHICS INFORMATION: 9 Drawing Sheet(s), 9 Figure(s).

DESCRIPTION OF FIGURES:

FIG. 1 illustrates an example of an amphiphile expected to be useful in encapsulating carbon nanotubes in accordance with the present invention;
FIG. 2 illustrates the predicted molecular structure of a selfassembled amphiphile around a carbon nanotube;
FIG. 3 illustrates another example of a amphiphile useful in accordance with the present invention;
FIG. 4 illustrates the general structure of a peptide amphiphile that self assembles and may be used to encapsulate carbon nanotubes in accordance with the present invention;
FIG. 5 illustrates another embodiment of a peptide-amphiphile useful in accordance with the present invention;
FIG. 6 is a photograph of single wall carbon nanotubes in: (a) flocculated water; (b) dispersed in water with the amphiphile of FIG. 7 of the present invention; and (c) dispersed in water with the amphiphile shown in FIG. 4 of the present invention capable of forming self assembled nanofibers.
FIG. 7 illustrates yet another example of an Amphiphile useful in the present invention.

AB This invention is directed to encapsulated nanotubes, methods of encapsulating carbon nanotubes, and uses for encapsulated nanotubes. Carbon nanotubes are encapsulated by self assembly of Uses of the present invention include making arrays as a basis for synthesis of carbon fibers.

NTE INDEXED FROM APPLICATION
Subject to any Disclaimer, the term of this patent is extended or adjusted under 35 USC 154(b) by 161 days.
CLMN 28
GI 9 Drawing Sheet(s), 9 Figure(s).
FIG. 1 illustrates an example of an amphiphile expected to be useful in encapsulating carbon nanotubes in accordance with the present invention;
FIG. 2 illustrates the predicted molecular structure of a selfassembled

amphiphile around a carbon nanotube;
FIG. 3 illustrates another example of a amphiphile useful in accordance with the present invention;
FIG. 4 illustrates the general structure of a peptide amphiphile that self assembles and may be used to encapsulate carbon nanotubes in accordance with the present invention;
FIG. 5 illustrates another embodiment of a peptide-amphiphile useful in accordance with the present invention;
FIG. 6 is a photograph of single wall carbon nanotubes in: (a) flocculated water; (b) dispersed in water with the amphiphile of FIG. 7 of the present invention; and (c) dispersed in water with the amphiphile shown in FIG. 4 of the present invention capable of forming self assembled nanofibers.
FIG. 7 illustrates yet another example of an Amphiphile useful in the present invention.

L11 ANSWER 6 OF 10 EMBASE COPYRIGHT (c) 2007 Elsevier B.V. All rights reserved on STN DUPLICATE 1

ACCESSION NUMBER: 2006114172 EMBASE
TITLE: Self-assembling peptide amphiphile nanofiber matrices for cell entrapment.
AUTHOR: Beniash E.; Hartgerink J.D.; Storrie H.; Stendahl J.C.; Stupp S.I.
CORPORATE SOURCE: S.I. Stupp, Department of Materials Science and Engineering, Chemistry and the Feinberg School of Medicine, Northwestern University, Evanston, IL 60208, United States. s-stupp@northwestern.edu
SOURCE: Acta Biomaterialia, (Jul 2005) Vol. 1, No. 4, pp. 387-397. Refs: 64
ISSN: 1742-7061
PUBLISHER IDENT.: S 1742-7061(05)00075-9
COUNTRY: United Kingdom
DOCUMENT TYPE: Journal; Article
FILE SEGMENT: 027 Biophysics, Bioengineering and Medical Instrumentation
029 Clinical and Experimental Biochemistry
LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 21 Mar 2006
Last Updated on STN: 21 Mar 2006

AB We have developed a class of peptide amphiphile (PA) molecules that self-assemble into three-dimensional nanofiber networks under physiological conditions in the presence of polyvalent metal ions. The assembly can be triggered by adding PA solutions to cell culture media or other synthetic physiological fluids containing polyvalent metal ions. When the fluids contain suspended cells, PA self-assembly entraps cells in the nanofibrillar matrix, and the cells survive in culture for at least three weeks. We also show that entrapment does not arrest cell proliferation and motility. Biochemical and ultrastructural analysis by electron microscopy indicate that entrapped cells internalize the nanofibers and possibly utilize PA molecules in their metabolic pathways. These results demonstrate that PA nanofibrillar matrices have the potential to be used for cell transplantation or other tissue engineering applications. .COPYRGT. 2005 Acta Materiala Inc. Published by Elsevier Ltd. All rights reserved.

L11 ANSWER 7 OF 10 DISSABS COPYRIGHT (C) 2007 ProQuest Information and Learning Company; All Rights Reserved on STN

ACCESSION NUMBER: 2005:39510 DISSABS Order Number: AAI3156650
TITLE: Cellular interactions with bio-inspired, nanoscale inorganic and organic materials for human repair
AUTHOR: Storrie, Hannah [Ph.D.]; Stupp, Samuel I. [advisor]
CORPORATE SOURCE: Northwestern University (0163)
SOURCE: Dissertation Abstracts International, (2004) Vol. 65, No.

12B, p. 6372. Order No.: AAI3156650. 192 pages.
ISBN: 0-496-17397-9.
DOCUMENT TYPE: Dissertation
FILE SEGMENT: DAI
LANGUAGE: English
ENTRY DATE: Entered STN: 20050826
Last Updated on STN: 20050826

AB This dissertation describes the use of engineered, nanoscale materials for human repair. Three different systems are discussed, one based on inorganic coatings for titanium substrates to be used for bone regeneration, and two based on self-assembling peptide amphiphile nanofibers that resemble the extra-cellular matrix. By controlling the chemistry and materials properties of the materials, specific cellular responses can be observed.

Organoapatite, a ceramic material containing hydroxyapatite, the mineral from which bone and teeth are make, and a small amount of poly(amino acids) has been chemically modified to adsorb zinc ions onto its surface. Zinc is an essential trace element found in bone and can stimulate biomineralization both in vitro and in vivo. When coated onto a titanium substrate via an electrostatic pretreatment, the new material, zinc-containing organoapatite (ZnOA), forms a porous, nanocrystalline material capable of delivering zinc ions to cells for biomineralization. In vitro studies of osteoblastic cells cultured on ZnOA coated titanium meshes in a rotating bioreactor show that ZnOA coatings promote the earlier onset of alkaline phosphatase (ALP) activity and the production of mineralized bone nodules as compared to controls.

Peptide amphiphile (PA) molecules containing a hydrophilic bioactive peptide head-group coupled to a hydrophobic alkyl tail that self-assemble to form nanofibers displaying the peptide head-group on the fiber have been studied as artificial extra cellular matrices. In one series of studies, the integrin-based adhesion of fibroblastic cells and the migration of highly invasive breast cancer cells on PA nanofibers containing the cell adhesion sequence RGDS was shown to be dependent on the architecture of the PA molecule. In another series of studies, PA's designed to mimic the active site of ALP displayed metal-dependent self-assembly, as well as specific binding of zinc ions to histidine residues in the PA and promoted the proliferation and biomineralization of osteoblastic cells.

L11 ANSWER 8 OF 10 IFIPAT COPYRIGHT 2007 IFI on STN
AN 10515509 IFIPAT;IFIUDB;IFICDB
TITLE: ENCAPSULATION OF NANOTUBES VIA SELF-ASSEMBLED NANOSTRUCTURES; FOR USE IN SYNTHESIS OF CARBON FIBERS
INVENTOR(S): Arnold; Michael Scott, Evanston, IL, US
Messmore; Benjamin W., Evanston, IL, US
Stupp; Samuel I., Chicago, IL, US
Zubarev; Eugene R., Ames, IA, US
PATENT ASSIGNEE(S): Unassigned
PATENT ASSIGNEE PROBABLE: Northwestern University (Probable)
AGENT: Pepper Hamilton LLP, One Mellon Center, 50th Floor, 500 Grant Street, Pittsburgh, PA, 15219, US

| | NUMBER | PK | DATE |
|---|---|---|---|
| PATENT INFORMATION: | US 2004022718 | A1 | 20040205 |
| APPLICATION INFORMATION: | US 2003-418474 | | 20030418 |

| | NUMBER | DATE |
|---|---|---|
| PRIORITY APPLN. INFO.: | US 2002-373827P | 20020418 (Provisional) |
| FAMILY INFORMATION: | US 2004022718 | 20040205 |
| | US 6890654 | 20050510 |

DOCUMENT TYPE: Utility
Patent Application - First Publication

FILE SEGMENT: CHEMICAL
APPLICATION
ENTRY DATE: Entered STN: 6 Feb 2004
Last Updated on STN: 12 May 2005

GOVERNMENT INTEREST:

(0002) The United States Government may have certain rights to this invention pursuant to work funded thereby at Northwestern University under grants from the National Science Foundation Grant No. EEC-0118025 W Main N602.

PARENT CASE DATA:

This application claims priority from U.S. Provisional Application Serial No. 60/373,827 filed Apr. 18, 2002 the contents of which are incorporated herein by reference in their entirety.

NUMBER OF CLAIMS: 29 7 Figure(s).
DESCRIPTION OF FIGURES:

FIG. 1 illustrates an example of an amphiphile expected to be useful in encapsulating carbon nanotubes in accordance with the present invention;
FIG. 2 illustrates the predicted molecular structure of a selfassembled amphiphile around a carbon nanotube;
FIG. 3 illustrates another example of a amphiphile useful in accordance with the present invention;
FIG. 4 illustrates the general structure of a peptide amphiphile that self assembles and may be used to encapsulate carbon nanotubes in accordance with the present invention;
FIG. 5 illustrates another embodiment of a peptide-amphiphile useful in accordance with the present invention;
FIG. 6 is a photograph of single wall carbon nanotubes in: (a) flocculated water; (b) dispersed in water with the amphiphile of FIG. 7 of the present invention; and (c) dispersed in water with the amphiphile shown in FIG. 4 of the present invention capable of forming self assembled nanofibers.
FIG. 7 illustrates yet another example of an Amphiphile useful in the present invention.

AB This invention is directed to encapsulated nanotubes, methods of encapsulating carbon nanotubes, and uses for encapsulated nanotubes. Carbon nanotubes are encapsulated by self assembly of Uses of the present invention include making arrays as a basis for synthesis of carbon fibers.

CLMN 29 7 Figure(s).

FIG. 1 illustrates an example of an amphiphile expected to be useful in encapsulating carbon nanotubes in accordance with the present invention;
FIG. 2 illustrates the predicted molecular structure of a selfassembled amphiphile around a carbon nanotube;
FIG. 3 illustrates another example of a amphiphile useful in accordance with the present invention;
FIG. 4 illustrates the general structure of a peptide amphiphile that self assembles and may be used to encapsulate carbon nanotubes in accordance with the present invention;
FIG. 5 illustrates another embodiment of a peptide-amphiphile useful in accordance with the present invention;
FIG. 6 is a photograph of single wall carbon nanotubes in: (a) flocculated water; (b) dispersed in water with the amphiphile of FIG. 7 of the present invention; and (c) dispersed in water with the amphiphile shown in FIG. 4 of the present invention capable of forming self assembled nanofibers.
FIG. 7 illustrates yet another example of an Amphiphile useful in the present invention.

L11 ANSWER 9 OF 10 IFIPAT COPYRIGHT 2007 IFI on STN
AN 10494693 IFIPAT;IFIUDB;IFICDB
TITLE: SELF-ASSEMBLY OF PEPTIDE-AMPHIPHILE NANOFIBERS UNDER PHYSIOLOGICAL CONDITIONS; GELATION OF POLYPEPTIDE BY

SOL, GEL PROCESS

INVENTOR(S): Béniash; Elia, Auburndale, MA, US
Hartgerink; Jeffrey D., Pearland, TX, US
Stupp; Samuel I., Chicago, IL, US
PATENT ASSIGNEE(S): Unassigned
PATENT ASSIGNEE PROBABLE: Northwestern University (Probable)
AGENT: REINHART BOERNER VAN DEUREN S.C. ATTN: LINDA GABRIEL, DOCKET COORDINATOR, 1000 NORTH WATER STREET, SUITE 2100, MILWAUKEE, WI, 53202, US

| | NUMBER | PK | DATE |
|---|---|---|---|
| PATENT INFORMATION: | US 2004001893 | A1 | 20040101 |
| APPLICATION INFORMATION: | US 2003-368517 | | 20030218 |

| | NUMBER | DATE |
|---|---|---|
| PRIORITY APPLN. INFO.: | US 2002-357228P | 20020215 (Provisional) |
| FAMILY INFORMATION: | US 2004001893 | 20040101 |

DOCUMENT TYPE: Utility
Patent Application - First Publication
FILE SEGMENT: CHEMICAL
APPLICATION
ENTRY DATE: Entered STN: 6 Jan 2004
Last Updated on STN: 7 Apr 2005

GOVERNMENT INTEREST:

(0002) The United States government has certain rights to this invention pursuant to Grant Nos. DE-FG02-00ER45810/A001, DMR9996253 and F49620-00-1-0283/P01 from, respectively, the DOE, NSF and AFOSR-MURI to Northwestern University.

PARENT CASE DATA:

This application claims priority benefit from U.S. provisional application Ser. No. 60/357,228 filed Feb. 15, 2002, the entirety of which is incorporated herein by reference.

NUMBER OF CLAIMS: 33 14 Figure(s).

DESCRIPTION OF FIGURES:

FIG. 1. In accordance with this invention: a) Chemical structure of a preferred peptide amphiphile, highlighting one or more structural features thereof. Region 1 may comprise a long alkyl tail that conveys hydrophobic character to the molecule and combined with the peptide region makes the molecule amphiphilic. Region 2 may comprise one or more (four consecutive, shown) cysteine residues which when oxidized may form disulfide bonds to provide a desired robust self-assembled structure. Region 3 may comprise a flexible linker region of one or more glycine residues, preferably three, or functionally similar such residues or monomers, to provide the hydrophilic head group flexibility from the more rigid crosslinked region. Region 4 may comprise a single phosphorylated serine residue which is designed to interact strongly with calcium ions and help direct mineralization of hydroxyapatite. Region 5 may comprise cell adhesion ligand RGD. b) Molecular model of an illustrated PA showing the overall conical shape of the molecule going from the narrow hydrophobic tail to the bulkier peptide region. c) Schematic showing the self-assembly of PA molecules into a cylindrical micelle.

FIG. 2. a) Negative stain (phosphotungstic acid) TEM of selfassembled nanofibers before covalent capture. Fibers are arranged in ribbon-like parallel arrays. b) Vitreous ice cryoTEM of the fibers reveals the diameter of the fibers in their native hydrated state to be 7.6+-1 nm. c) Positive stain (uranyl acetate) TEM of the self-assembled nanofibers after oxidative cross-linking showing electron dense regions due to the stain that localized on the periphery of the fibers. d) Thin section TEM of positively stained (uranyl acetate) nanofibers after oxidative cross-linking and embedding in epoxy resin.

Two fibers are observed in cross-section (arrows) clearly showing the lack of staining in the interior of the fiber.
FIG. 3. a) TEM micrographs of the unstained, cross-linked peptide-amphiphile fibers incubated for 10 min in CaCl2 and Na2HPO4 solution. The fibers arranged in bundles are visible due to the high concentration of inorganic ions on their surface. b) After 20 minutes forming HA crystals (arrows) are observed in parallel arrays on some of the PA fibers. c) After 30 minutes mature HA crystals (arrows) completely cover the PA fibers. d) Electron diffraction pattern taken from a mineralized bundle of PA fibers after 30 minutes of exposure to calcium and phosphate. The presence and orientation of the diffraction arcs corresponding to the 002 and 004 planes indicate preferential alignment of the crystals with their caxes along the long axis of the bundle. e) Plot of intensity versus inverse angstroms reveals that the 002 and 004 peaks of hydroxyapatite are strongly enhanced along the peptideamphiphile fiber axis. f) EDS profile of mineral crystals after 30 minutes of incubation reveals a Ca/P ratio of 1.67+/-0.08 as expected for HA.
FIG. 4. Scheme showing possible relationships between peptideamphiphile fibers and hydroxyapatite crystals in the mineralized bundle. Arrow indicates the direction of the c-axes of the crystals.
FIG. 5. A tilt pair taken from mineralized PA fibers after 30 minutes of incubation with calcium and phosphate demonstrating the plate shape of the crystals. The crystals that were "edgeon" (electron dense, narrow objects) in the zero degree image lose contrast in the 45 degree rotated image (arrow 1) while the contrast of the crystals that were "face-on" in the zero degree images increase (arrow 2).
FIG. 6. a) Nonphosphorylated PA fibers after 20 minutes of incubation with calcium and phosphate shows only amorphous mineral deposit concentrate on the fibers. b) Nonphosphorylated PA after 30 minutes of incubation with calcium and phosphate continue to show only amorphous mineral in contrast with phosphorylated PA which shows heavy crystallization at this time point.
FIGS. 7-9. TEM micrographs for several cylindrical micelles prepared from PA molecules listed in Table 1. Specifically: FIG. 7, Top: Molecule #4 containing a C10 alkyl tail. Bottom: Molecule #13 containing a C22 alkyl tail; FIG. 8, Top: Molecule 8 utilizing a tetra alanine sequence in place of tetra cysteine and containing a C16 alkyl tail. Bottom: Molecule 9 utilizing a tetra alanine sequence in place of tetra cysteine and containing a C10 alkyl tail; and FIG. 9, peptide-amphiphiles with three different peptide head groups. Top: Molecule 10 with "KGE". Middle: Molecule 14 lacking the phosphoserine group. Bottom: Molecule 15 with "IKVAV."
FIGS. 10A-B. Chemical structures of PA compositions 21 and 22, with reference to Table 2, below.
FIGS. 10C-E. Chemical structures of four peptide-amphiphiles used for self-assembly.
FIG. 11. Molecule 1 self-assemblies into nanofibers upon drying from a solution at physiological pH.
FIG. 12. TEM micrographs of positively stained peptideamphiphile gels formed by addition of: A) Ca+2 to molecule 2 solution; B) Cd+2 and molecule 2 solution; C) Ca+2 to molecule 4 solution; D) Fe+2 to molecule 1 solution; and e) Zn+2 to molecule 1 solution.
FIG. 13. Self-assembly induced by mixing two different peptide amphipiles (21 and 22) containing opposite charges.
FIGS. 14A-C. TEM images of three different self-assembled peptide-amphiphile nanofibers. 14A: Negatively charged peptide amphiphile 25 assembled with acid. 14B: Positively charged 24 assembled with base. 14C: Nanofibers formed at neutral pH with a mixture of 24 and 25.
FIGS. 15A-C. FT-IR spectra of the peptide-amphiphile gels. A. The fragment of the spectrum of CaCl2 induced gel of the molecule 27, showing the regions of Amide A, Amide I and Amide II bands. B. The Amide I and II region of the normalized spectra of the gels of the molecule 27 assemblied by addition of CaCl2 and at low pH. C. The Amide I and II region of the normalized spectra of the gels of the molecule 32 assemblied by addition of CaCl2, pH and KCl.
AB Peptide amphiphile compounds, compositions and methods for selfassembly or nanofibrous network formation under neutral or physiological conditions.

CLMN 33 14 Figure(s).

FIG. 1. In accordance with this invention: a) Chemical structure of a preferred peptide amphiphile, highlighting one or more structural features thereof. Region 1 may comprise a long alkyl tail that conveys hydrophobic character to the molecule and combined with the peptide region makes the molecule amphiphilic. Region 2 may comprise one or more (four consecutive, shown) cysteine residues which when oxidized may form disulfide bonds to provide a desired robust self-assembled structure. Region 3 may comprise a flexible linker region of one or more glycine residues, preferably three, or functionally similar such residues or monomers, to provide the hydrophilic head group flexibility from the more rigid crosslinked region. Region 4 may comprise a single phosphorylated serine residue which is designed to interact strongly with calcium ions and help direct mineralization of hydroxyapatite. Region 5 may comprise cell adhesion ligand RGD. b) Molecular model of an illustrated PA showing the overall conical shape of the molecule going from the narrow hydrophobic tail to the bulkier peptide region. c) Schematic showing the self-assembly of PA molecules into a cylindrical micelle.

FIG. 2. a) Negative stain (phosphotungstic acid) TEM of selfassembled nanofibers before covalent capture. Fibers are arranged in ribbon-like parallel arrays. b) Vitreous ice cryoTEM of the fibers reveals the diameter of the fibers in their native hydrated state to be 7.6+-1 nm. c) Positive stain (uranyl acetate) TEM of the self-assembled nanofibers after oxidative cross-linking showing electron dense regions due to the stain that localized on the periphery of the fibers. d) Thin section TEM of positively stained (uranyl acetate) nanofibers after oxidative cross-linking and embedding in epoxy resin. Two fibers are observed in cross-section (arrows) clearly showing the lack of staining in the interior of the fiber.

FIG. 3. a) TEM micrographs of the unstained, cross-linked peptide-amphiphile fibers incubated for 10 min in CaCl2 and Na2HPO4 solution. The fibers arranged in bundles are visible due to the high concentration of inorganic ions on their surface. b) After 20 minutes forming HA crystals (arrows) are observed in parallel arrays on some of the PA fibers. c) After 30 minutes mature HA crystals (arrows) completely cover the PA fibers. d) Electron diffraction pattern taken from a mineralized bundle of PA fibers after 30 minutes of exposure to calcium and phosphate. The presence and orientation of the diffraction arcs corresponding to the 002 and 004 planes indicate preferential alignment of the crystals with their caxes along the long axis of the bundle. e) Plot of intensity versus inverse angstroms reveals that the 002 and 004 peaks of hydroxyapatite are strongly enhanced along the peptideamphiphile fiber axis. f) EDS profile of mineral crystals after 30 minutes of incubation reveals a Ca/P ratio of 1.67+/-0.08 as expected for HA.

FIG. 4. Scheme showing possible relationships between peptideamphiphile fibers and hydroxyapatite crystals in the mineralized bundle. Arrow indicates the direction of the c-axes of the crystals.

FIG. 5. A tilt pair taken from mineralized PA fibers after 30 minutes of incubation with calcium and phosphate demonstrating the plate shape of the crystals. The crystals that were "edgeon" (electron dense, narrow objects) in the zero degree image lose contrast in the 45 degree rotated image (arrow 1) while the contrast of the crystals that were "face-on" in the zero degree images increase (arrow 2).

FIG. 6. a) Nonphosphorylated PA fibers after 20 minutes of incubation with calcium and phosphate shows only amorphous mineral deposit concentrate on the fibers. b) Nonphosphorylated PA after 30 minutes of incubation with calcium and phosphate continue to show only amorphous mineral in contrast with phosphorylated PA which shows heavy crystallization at this time point.

FIGS. 7-9. TEM micrographs for several cylindrical micelles prepared from PA molecules listed in Table 1. Specifically: FIG. 7, Top: Molecule #4 containing a C10 alkyl tail. Bottom: Molecule #13 containing a C22 alkyl tail; FIG. 8, Top: Molecule 8 utilizing a tetra alanine sequence in place of tetra cysteine and containing a C16 alkyl tail. Bottom: Molecule 9

utilizing a tetra alanine sequence in place of tetra cysteine and containing a C10 alkyl tail; and FIG. 9, peptide-amphiphiles with three different peptide head groups. Top: Molecule 10 with "KGE". Middle: Molecule 14 lacking the phosphoserine group. Bottom: Molecule 15 with "IKVAV."

FIGS. 10A-B. Chemical structures of PA compositions 21 and 22, with reference to Table 2, below.

FIGS. 10C-E. Chemical structures of four peptide-amphiphiles used for self-assembly.

FIG. 11. Molecule 1 self-assemblies into nanofibers upon drying from a solution at physiological pH.

FIG. 12. TEM micrographs of positively stained peptideamphiphile gels formed by addition of: A) Ca+2 to molecule 2 solution; B) Cd+2 and molecule 2 solution; C) Ca+2 to molecule 4 solution; D) Fe+2 to molecule 1 solution; and e) Zn+2 to molecule 1 solution.

FIG. 13. Self-assembly induced by mixing two different peptide amphipiles (21 and 22) containing opposite charges.

FIGS. 14A-C. TEM images of three different self-assembled peptide-amphiphile nanofibers. 14A: Negatively charged peptide amphiphile 25 assembled with acid. 14B: Positively charged 24 assembled with base. 14C: Nanofibers formed at neutral pH with a mixture of 24 and 25.

FIGS. 15A-C. FT-IR spectra of the peptide-amphiphile gels. A. The fragment of the spectrum of CaCl2 induced gel of the molecule 27, showing the regions of Amide A, Amide I and Amide II bands. B. The Amide I and II region of the normalized spectra of the gels of the molecule 27 assemblied by addition of CaCl2 and at low pH. C. The Amide I and II region of the normalized spectra of the gels of the molecule 32 assemblied by addition of CaCl2, pH and KCl.

L11 ANSWER 10 OF 10 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 2003-712608 [67] WPIDS
CROSS REFERENCE: 2005-081949
DOC. NO. CPI: C2003-195983 [67]
TITLE: Sol-gel system used for e.g. tissue engineering comprises peptide amphiphile compound having bioactive epitope sequence, hydrophobic component and reagent to induce gelation of amphiphile compound
DERWENT CLASS: B04; B07
INVENTOR: BENIASH E; HARTGERINK J D; STUPP S I
PATENT ASSIGNEE: (BENI-I) BENIASH E; (HART-I) HARTGERINK J D; (STUP-I) STUPP S I; (NOUN-C) UNIV NORTHWESTERN
COUNTRY COUNT: 30

PATENT INFO ABBR.:

| PATENT NO | KIND | DATE | WEEK | LA | PG | MAIN IPC |
|---|---|---|---|---|---|---|
| WO 2003070749 | A2 | 20030828 | (200367)* | EN | 27[0] | |
| US 20040001893 | A1 | 20040101 | (200402) | EN | | |
| AU 2003215280 | A1 | 20030909 | (200427) | EN | | |
| AU 2003215280 | A8 | 20051027 | (200629) | EN | | |

APPLICATION DETAILS:

| PATENT NO | KIND | APPLICATION | DATE |
|---|---|---|---|
| WO 2003070749 | A2 | WO 2003-US4779 | 20030218 |
| US 20040001893 | A1 Provisional | US 2002-357228P | 20020215 |
| AU 2003215280 | A1 | AU 2003-215280 | 20030218 |
| US 20040001893 | A1 | US 2003-368517 | 20030218 |
| AU 2003215280 | A8 | AU 2003-215280 | 20030218 |

FILING DETAILS:

| PATENT NO | KIND | | PATENT NO | |
|---|---|---|---|---|
| AU 2003215280 | A1 | Based on | WO 2003070749 | A |
| AU 2003215280 | A8 | Based on | WO 2003070749 | A |

PRIORITY APPLN. INFO: US 2002-357228P 20020215
US 2003-368517 20030218
AN 2003-712608 [67] WPIDS
CR 2005-081949
AB WO 2003070749 A2 UPAB: 20050904
NOVELTY - Sol-gel system comprises a peptide amphiphile compound (A) having a bioactive epitope sequence, a hydrophobic component (B) and a reagent (C) to induce gelation of (A).

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for:

(1) formation of a peptide amphiphile nanofiber which comprises placing an aqueous medium containing (A) and (B) on a surface and removing the aqueous component from the medium, or introducing a reagent to the medium to induce nanofiber formation, and

(2) a peptide amphiphile composition which comprises a hydrophobic group and a first (a1) and a second (a2) amino acid sequence having a first and a second bioactive epitope sequence, respectively. (a1) And (a2) have charges opposite to each other at a physiological pH.

USE - Used in biomedical applications e.g. in vivo or in vitro delivery of cells, drugs or therapeutic agent, in cell therapies and in tissue engineering, and to obtain cell and/or mineral growth onto a variety of hard and soft biomimetic materials for biological and non-biological applications (e.g. catalysis, photonics and electronics).

ADVANTAGE - The peptide amphiphile component is stable at physiological pH with or without covalent crosslinking. The system forms a facile self assembly of nanostructured fiber under a physiological pH condition. The system avoids contact between tissues and the material sensitive to pH change at non-physiological pH.

=> s (peptide? or polypeptide? or protein?) (P) (nanofiber? or nanostructure? or nanotube? or nanoparticle? or nanocluster? ) (P) metal?
L12 713 FILE IFIPAT
L13 754 FILE CAPLUS
L14 79 FILE DISSABS
L15 322 FILE SCISEARCH
L16 106 FILE EMBASE
L17 42 FILE LIFESCI
L18 167 FILE MEDLINE
L19 565 FILE WPIDS

TOTAL FOR ALL FILES
L20 2748 (PEPTIDE? OR POLYPEPTIDE? OR PROTEIN?) (P) (NANOFIBER? OR NANOSTRUCTURE? OR NANOTUBE? OR NANOPARTICLE? OR NANOCLUSTER? ) (P) METAL?

=> s (peptide? or polypeptide? or protein?) (s) (nanofiber? or nanostructure? or nanotube? or nanoparticle? or nanocluster? ) (P) metal?
L21 292 FILE IFIPAT
L22 536 FILE CAPLUS
L23 61 FILE DISSABS
L24 177 FILE SCISEARCH
L25 66 FILE EMBASE
L26 41 FILE LIFESCI
L27 104 FILE MEDLINE
L28 379 FILE WPIDS

TOTAL FOR ALL FILES
L29 1656 (PEPTIDE? OR POLYPEPTIDE? OR PROTEIN?) (S) (NANOFIBER? OR NANOSTRUCTURE? OR NANOTUBE? OR NANOPARTICLE? OR NANOCLUSTER? ) (P)

METAL?

=>
<------User Break------>

=> s peptide? (w) (nanofiber? or nanostructure? or nanotube? or nanoparticle? or nanocluster? ) (P) metal?
L30 5 FILE IFIPAT
L31 33 FILE CAPLUS
L32 4 FILE DISSABS
L33 19 FILE SCISEARCH
L34 4 FILE EMBASE
L35 3 FILE LIFESCI
L36 6 FILE MEDLINE
L37 2 FILE WPIDS

TOTAL FOR ALL FILES
L38 76 PEPTIDE? (W) (NANOFIBER? OR NANOSTRUCTURE? OR NANOTUBE? OR NANOP ARTICLE? OR NANOCLUSTER? ) (P) METAL?

=> dep rem l38
DEP IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> dup rem l38
PROCESSING COMPLETED FOR L38
L39 53 DUP REM L38 (23 DUPLICATES REMOVED)

=> d l39 40-53 ibib abs

L39 ANSWER 40 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:636003 CAPLUS
TITLE: Size-, packing density-, and shape-controlled nanocrystal-coated nanotube fabrication using molecular recognition and conformation control of sequenced peptides
AUTHOR(S): Banerjee, Ipsita A.; Yu, Lingtao; Matsui, Hiroshi
CORPORATE SOURCE: Department of Chemistry, The City University of New York, Hunter College, New York, NY, 10021, USA
SOURCE: Abstracts of Papers, 226th ACS National Meeting, New York, NY, United States, September 7-11, 2003 (2003), PHYS-102. American Chemical Society: Washington, D. C.
CODEN: 69EKY9
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB With recent interest in seeking new biol. inspired, device fabrication methods for nanotechnol., we are developing a new biol. approach to fabricate metal nanowires by using sequenced peptide nanotubes as templates. The sequenced peptide mols. were assembled as nanotubes and the biol. recognition of the sequenced peptide toward metals lead to efficient metal nanocrystal coatings such as Au, Ag, Cu, Ni on the nanowires. Highly crystalline metal nanocrystals were uniformly coated on the peptide nanotubes with the high-d. coverage. The conformations and the charge distributions of the sequenced peptide on surfaces, determined by pH and ion concns. in the growth solns., control the size and the packing d. of nanocrystals. In the case of Ag nanocrystals, the shape of nanocrystals was also controlled. It should be noted that metallic nanocrystals in diameter around 6 nm are in the size domain to observe significant conductivity change by changing the packing d., and therefore this system may be developed to a conductivity-tunable building block. We believe

this simple metal nanowire fabrication method can be applied to various metals and semiconductors with peptides whose sequences are known to mineralize specific ions.

L39 ANSWER 41 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:185816 CAPLUS
TITLE: Fabrication of Au nanowires on peptide nanotubes by tuning sequenced peptide conformations
AUTHOR(S): Matsui, Hiroshi; Djalali, Ramin; Chen, Yung-fu
CORPORATE SOURCE: Department of Chemistry, City University of New York, Hunter College, New York, NY, 10021, USA
SOURCE: Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), PMSE-017. American Chemical Society: Washington, D. C.
CODEN: 69DSA4
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB A new biol. approach to fabricate Au nanowires was examined by using sequenced histidine-rich peptide nanowires as templates. The sequenced histidine-rich peptide mols. were assembled as nanowires, and the biol. recognition of the sequenced peptide toward Au lead to efficient Au coating on the nanowires. Monodisperse Au nanocrystals were uniformly coated on the histidine peptide nanowires with the high-d. coverage. The uniformity of the Au coating on the nanowires without contamination of precipitated Au aggregates is advantageous for the fabrication of electronics and sensor devices when the nanowires are used as the building blocks. We believe this simple metal nanowire fabrication method can be applied to various metals and semiconductors with peptides whose sequences are known to mineralize specific ions. Figure show TEM images of the sequenced histidine-rich peptide nanotube (l.) and Au on the nanowire coated with the sequenced histidine-rich peptide (r.) Inset shows the Au-nanocrystals with a diameter of 6nm.

L39 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 9
ACCESSION NUMBER: 2003:668879 CAPLUS
DOCUMENT NUMBER: 140:299602
TITLE: Biomolecular applications of carbon nanotubes
AUTHOR(S): Baxendale, M.
CORPORATE SOURCE: Physics Department, Queen Mary, University of London, London, E1 4NS, UK
SOURCE: IEE Proceedings: Nanobiotechnology (2003), 150(1), 3-8
CODEN: IPNEAY; ISSN: 1478-1581
PUBLISHER: Institution of Electrical Engineers
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. Carbon nanotubes are a significant addition to the emerging field of nanotube biotechnol. The biocompatibility, high structural integrity, and unique electronic and mech. properties of carbon nanotubes complement or surpass those of self-assembled lipid nanotubes, peptide nanotubes, and template-synthesized nanotubes (metals, polymers, semiconductors, and carbons). Carbon nanotubes are candidates for a range of biomol. applications that is likely to widen considerably in the future.
REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 43 OF 53 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 2002:723548 SCISEARCH
THE GENUINE ARTICLE: 587QE
TITLE: Novel flexible frameworks of porous cobalt(III) coordination polymers that show selective guest adsorption

based on the switching of hydrogen-bond pairs of amide groups

AUTHOR: Uemura K; Kitagawa S (Reprint); Kondo M; Fukui K; Kitaura R; Chang H C; Mizutani T

CORPORATE SOURCE: Kyoto Univ, Grad Sch Engn, Dept Synthet Chem & Biol Chem, Sakyo Ku, Kyoto 6068501, Japan (Reprint); Reg Joint Res Project Yamagata Prefecture, Yamagata 9902473, Japan

COUNTRY OF AUTHOR: Japan

SOURCE: CHEMISTRY-A EUROPEAN JOURNAL, (16 AUG 2002) Vol. 8, No. 16, pp. 3586-3600.
ISSN: 0947-6539.

PUBLISHER: WILEY-V C H VERLAG GMBH, PO BOX 10 11 61, D-69451 WEINHEIM, GERMANY.

DOCUMENT TYPE: Article; Journal

LANGUAGE: English

REFERENCE COUNT: 92

ENTRY DATE: Entered STN: 20 Sep 2002
Last Updated on STN: 20 Sep 2002

*ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS*

AB Four porous crystalline coordination polymers with two-dimensional frameworks of a double-edged axe-shaped motif, {[Co(NCS)(2)(3-pia)(2)] . 2EtOH . 11 H2O}(n) (1a), {[Co(NCS)(2)- (3-pia)(2)] . 4Me(2)CO}(n) (3a), {[Co(NCS)(2)- (3-pia)(2)] . 4THF}(n) (3b) and {[Co(NCS)(2)-(3-pna)(2)](n)} (5), have been synthesized by the reaction of cobalt(ii) thiocyanate with N-(3-pyridyl)isonicotinamide (3-pia) or N-(3-pyridyl)nicotinamide (3-pna). X-ray crystallographic characterization reveals that adjacent layers are stacked such that channels are created, except in 5. The channels form a hydrogen-bonded interior for guest molecules; in practice, I a contains ethanol and water molecules as guests in the channels with hydrogen bonds, whereas 3b (3a) contains tetrahydrofuran (acetone) molecules. In la, the "double-edged axe-shaped" motifs in adjacent sheets are not located over the top of each other, while the motifs in 3b stack so perfectly as to overlap each other in an edge-to-edge fashion. This subtle change in the three-dimensional framework is associated with the template effect of the guests. Compound 5 has no guest molecules and, therefore, the amide groups in one sheet are used for hydrogen-bonding links with adjacent sheets. Removal of the guest molecules from la and 3b (3a) causes a structural conversion accompanied by a color change. Pink 1 a cannot retain its original framework and changes into a blue amorphous compound. On the other hand, the framework of pink 3b (3a) is transformed to a new crystalline framework of violet 4. Interestingly, 4 reverts to the original pink crystals of 3b (3a) when it is exposed to THF (or acetone) vapor. Spectroscopic measurements (visible, EPR, and IR) provide a clue to the crystal-to-crystal transformation; on removal of the guests, the amide groups are used to form the P sheet-type hydrogen bonding between the sheets, and thus the framework withstands significant stress on removal of guest molecules. This mechanism is attributed to the arrangement of the adjacent sheets so suited in regularity that the P sheet-type structure forms efficiently. The apohost 4 does not adsorb cyclopentane, showing a guest selectivity that, in addition to size, hydrogen-bonding capability is required for the guest molecules. The obtained compound is categorized as a member of a new generation of compounds tending towards functional porous coordination polymers.

L39 ANSWER 44 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:625025 CAPLUS

DOCUMENT NUMBER: 137:338554

TITLE: Self-assembly strategies for organic and hybrid nanomaterials

AUTHOR(S): Stupp, Samuel I.

CORPORATE SOURCE: Department of Materials Science and Engineering, Northwestern University, USA

SOURCE: Polymer Preprints (American Chemical Society, Division

of Polymer Chemistry) (2002), 43(2), 385
CODEN: ACPPAY; ISSN: 0032-3934
PUBLISHER: American Chemical Society, Division of Polymer Chemistry
DOCUMENT TYPE: Journal; (computer optical disk)
LANGUAGE: English
AB Self-assembly and templating are discussed as general strategies to create nanostructured organic and hybrid materials, in some cases combined with external forces such as elec. fields. One of the examples to be discussed is the self assembly of peptide nanofibers in water with the capacity to nucleate and organize hydroxyapatite crystals in a fashion that recreates the nanostructure of bone. In another example metal oxide nanocrystals are aligned by self assembling organic nanoribbons and weak elec. fields to produce effective UV lasing materials. A third example to be discussed is the templating of II-VI semiconductors by the same nanoribbons resulting in objects such as nanoscale helixes and double helixes.

L39 ANSWER 45 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:232545 CAPLUS
DOCUMENT NUMBER: 142:6770
TITLE: Self-assembled peptide nanotube: assembling mechanism and fabrications
AUTHOR(S): Matsui, Hiroshi
CORPORATE SOURCE: Department of Chemistry, City University of New York, New York, NY, 10021, USA
SOURCE: Recent Research Developments in Physical Chemistry (2002), 6(Pt. 2), 351-370
CODEN: RRPCFK
PUBLISHER: Transworld Research Network
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. This article introduces a new nanotube assembled by peptide mols., which can be applied to nano-fabrication techniques such as metalization, surface immobilization and nanocrystal coating due to its functionalities. The characteristic structural transformation of the peptide nanotubes between helical and tubule forms has potential to be applied to controlled releases.
REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 46 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:777372 CAPLUS
TITLE: Self-assembly strategies for organic and hybrid nanomaterials
AUTHOR(S): Stupp, Samuel I.
CORPORATE SOURCE: Department of Materials Science and Engineering, Department of Chemistry, Medical School, Northwestern University, Evanston, IL, 60208, USA
SOURCE: Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States, August 18-22, 2002 (2002), POLY-349. American Chemical Society: Washington, D. C.
CODEN: 69CZPZ
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB Self assembly is currently the only practical approach to synthesis of nanostructured organic materials. When combined with the use of external forces and top down patterning, its potential to create functional materials could be far reaching. In this lecture self-assembly and templating are discussed as general strategies to create nanostructured organic and hybrid materials, in some cases combined with external forces such as elec. fields. One of the examples to be discussed is the self assembly of peptide nanofibers in water with the

capacity to nucleate and organize hydroxyapatite crystals in a fashion that recreates the nanostructure of bone. In another example metal oxide nanocrystals are aligned by self assembling organic nanoribbons and weak elec. fields to produce effective UV lasing materials. A third example to be discussed is the templating of II-VI semiconductors by the same nanoribbons resulting in objects such as nanoscale helixes and double helixes.

L39 ANSWER 47 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:545770 CAPLUS
DOCUMENT NUMBER: 137:228340
TITLE: Immunoreactivity and characterization of histidine-rich peptide encapsulated nanoclusters
AUTHOR(S): Slocik, Joseph M.; Moore, Joshua T.; Wright, David W.
CORPORATE SOURCE: Department of Chemistry, Vanderbilt University, Nashville, TN, 37235-1822, USA
SOURCE: Materials Research Society Symposium Proceedings (2002), 711(Advanced Biomaterials: Characterization, Tissue Engineering and Complexity), 339-344
CODEN: MRSPDH; ISSN: 0272-9172
PUBLISHER: Materials Research Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Histidine-rich proteins (HRP), which function in the biol. control of inorg. materials, have been identified in the liver fluke Fasciola hepatica, marine polychaetes, humans, and the malarial parasite Plasmodium falciparum. For example, the malarial parasite contains HRP II composed of repeating peptide sequences of Ala-His-His-Ala-His-His-Ala-Ala-Asp. This peptide was screened as a stabilizing peptide coat for a variety of nanoclusters of Ag0, Au0, ZnS, TiO2, and Ag2S, and characterized by UV-Vis spectroscopy, fluorescence, IR, XRD, and TEM. The resulting nanoclusters were examined for immunoreactivity against a com. monoclonal antibody for HRP II of P. falciparum.
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 48 OF 53 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 2001:957414 SCISEARCH
THE GENUINE ARTICLE: 497CE
TITLE: Ionic channel structures in [(M+)(x)([18]crown-6)][Ni(dmit)(2)](2) molecular conductors
AUTHOR: Akutagawa T (Reprint); Hasegawa T; Nakamura T; Takeda S; Inabe T; Sugiura K; Sakata Y; Underhill A E
CORPORATE SOURCE: Hokkaido Univ, Res Inst Elect Sci, Sapporo, Hokkaido 0600812, Japan (Reprint); Hokkaido Univ, Fac Sci, Dept Chem, Sapporo, Hokkaido 0600810, Japan; Osaka Univ, Inst Sci & Ind Res, Ibaraki, Osaka 5670047, Japan; Univ Wales, Dept Chem, Bangor LL57 3UW, Gwynedd, Wales
COUNTRY OF AUTHOR: Japan; Wales
SOURCE: CHEMISTRY-A EUROPEAN JOURNAL, (19 NOV 2001) Vol. 7, No. 22, pp. 4902-4912.
ISSN: 0947-6539.
PUBLISHER: WILEY-V C H VERLAG GMBH, PO BOX 10 11 61, D-69451 BERLIN, GERMANY.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 84
ENTRY DATE: Entered STN: 14 Dec 2001
Last Updated on STN: 14 Dec 2001
*ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS*
AB The [(M+),([18]crown-6)] supramolecular cations (SC), in which M+ and [18]crown-6 are alkali metal ions (M+ = Li+, Na+, and Cs+), and 1,4,7,10,13, 16-hexaoxacyclooctadecane, respectively, form ionic channel

structures through the regular stacks of [18]crown-6 in [Ni(dmit)(2)]-based molecular conductors (dmit(2) =2-thioxo-1,3-dithiole-4,5-dithiolate). In addition to the [Ni(dmit)(2)] salts that have the ionic channel structures (these salts are abbreviated as type I salts), Li+ and Na+ form dimerized [(M+)(2)([18]crown-6)(2)] units in the crystals (type II salts). The K+ and Rb+ are coordinated tightly into the [18]crown-6 cavity to form typical diskshape SC+ units in the corresponding [Ni(dmit)(2)] salts (type III salts). The type I, II, and III salts have typical stoichiometries of [(M+),([18]crown-6)]-[Ni(dmit)(2)](2), [(M+)([18]crown-6)(H2O)(x),(CH3CN)(1.5-x)][Ni(dmit)(2)](3) (x = 1 for Li+ or 0.5 for Na+). and [M+([18]crown-6)][Ni(dmit)(2)](3), respectively; the salts of the same type are isostructural. In agreement with the trimer structures of [Ni(dmit)(2)] in the type II and III salts, they exhibit semiconducting behavior with electrical conductivities at 300 K (sigma (300K) of 0.01 - 0.1 S cm(-1). Type I salts contain a regular stack of partially oxidized [Ni(dmit)(2)] units, which form a quasi one-dimensional metallic band within the tight-binding approximation regime. The electrical conductivities at 300 K are 10 - 30 S cm(-1), and an almost temperature-independent conductivity was observed at higher temperatures, However, the one-dimensional electronic structures in these salts are strongly influenced by the static and dynamic structures of the coexisting ionic channel. The Na+ salt is a semiconductor, whose magnetic behavior is described by the disordered one-dimensional antiferromagnetic chain. On the other hand, the Cs+ salt is a exhibits metallic properties with 2k(P) instability at room temperature. The Li+ salt shows a gradual transition from the high-temperature metallic phase to the low-temperature one-dimensional antiferromagnetic semiconductor phase, which was associated with the freezing of Li+ motion at lower temperatures. The preferential crystallization of type I salts was possible by controlling the equilibrium constant (K-c) of the complex formation between M+ ions and the [18]crown-6 molecule. The ionic channel structures were obtained when the K-c was low in the electrocrystallization solution, while type II or III salts were formed in the high K-c region.

L39 ANSWER 49 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 10

ACCESSION NUMBER: 2001:754445 CAPLUS
DOCUMENT NUMBER: 136:43410
TITLE: Metalloporphyrin Nanotube Fabrication Using Peptide Nanotubes as Templates
AUTHOR(S): Matsui, Hiroshi; MacCuspie, Robert
CORPORATE SOURCE: Department of Chemistry, Hunter College, City University of New York, New York, NY, 10021, USA
SOURCE: Nano Letters (2001), 1(12), 671-675
CODEN: NALEFD; ISSN: 1530-6984
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Protoporphyrin IX Zn(II) forms metalloporphyrin coatings on peptide nanotubes via hydrogen bonds and produce metalloporphyrin nanotubes. This diacid metalloporphyrin was stabilized on the peptide nanotube surfaces with two types of hydrogen bonds, intermol. hydrogen bond between the carboxylic acid of metalloporphyrins and the amide of peptide nanotube and intermol. hydrogen bond between the carboxylic acids of neighboring metalloporphyrins. Since previous study indicates that the peptide nanotubes can potentially be assembled as arrays, the applications of metalloporphyrin nanotubes to nanoscale chemical sensors or photonics may be possible.
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 50 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 11

ACCESSION NUMBER: 2001:849478 CAPLUS
DOCUMENT NUMBER: 136:127017
TITLE: Controlled immobilization of peptide nanotube-templated metallic wires on Au surfaces
AUTHOR(S): Matsui, H.; Gologan, B.; Pan, S.; Douberly, G. E., Jr.
CORPORATE SOURCE: Department of Chemistry, University of Central Florida, Orlando, FL, 32816, USA
SOURCE: European Physical Journal D: Atomic, Molecular and Optical Physics (2001), 16(1-3), 403-406
CODEN: EPJDF6; ISSN: 1434-6060
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Peptide nanotubes were immobilized on Au substrates functionalized with self-assembled monolayers of 4-mercaptobenzoic acid in a pH 6 citric acid solution via hydrogen bonds between the peptide nanotubes and the monolayers. Subsequently, the immobilized nanotubes were metalized by nickel via the electroless coating process.
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 51 OF 53 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 2000:366372 SCISEARCH
THE GENUINE ARTICLE: 312NZ
TITLE: Toward artificial ion channels: A lipophilic G-quadruplex
AUTHOR: Forman S L; Fettinger J C; Pieraccini S; Gottareli G; Davis J T (Reprint)
CORPORATE SOURCE: Univ Maryland, Dept Chem & Biochem, College Pk, MD 20742 USA (Reprint); Univ Bologna, Dipartimento Chim Organ A Mangini, I-40127 Bologna, Italy
COUNTRY OF AUTHOR: USA; Italy
SOURCE: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, (3 MAY 2000) Vol. 122, No. 17, pp. 4060-4067.
ISSN: 0002-7863.
PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 91
ENTRY DATE: Entered STN: 2000
Last Updated on STN: 2000
*ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS*

AB Single crystals of a lipophilic G-quadruplex formed by 5'-tert-butyl-dimethylsilyl-2',3',-di-O-isopropylidene G 2 were obtained from a CH3CN solution containing potassium picrate and cesium picrate. The X-ray structure showed that 16 units of G 2 and 4 equiv of alkali picrate form the lipophilic G-quadruplex. The quadruplex has a filled cation channel, with three K+ ions and one Cs+ ion located along its central axis. The quadruplex is formed by a pair of head-to-tail (G 2)(8)-K+ octamers. Both octamers use eight carbonyl oxygens to coordinate K+. The two (G 2)(8)-K+ octamers are of opposite polarity, being coaxially stacked in a head-to-head orientation. A Cs+ cation, with an unusual coordination geometry, caps the cation channel. The Cs+ is coordinated to four acetonitrile solvent molecules in an eta(2)-fashion. Within an octamer the two tetramers are stacked so that they are 3.3 Angstrom apart and twisted by 30 degrees. A second stacking interaction is defined by the bend-to-head arrangement between the two (G 2)(8)-K+ octamers. This stacking, with a 90 degrees twist, positions the exocyclic amines of the central two quartets so that both exocyclic NH2(B) protons can hydrogen bond to the picrate anions that rim the quadruplex equator. The four picrates form an anionic belt that wraps around the cation

channel. The sugars are well ordered in the structure. Circular dichroism spectra indicate that the G-quadruplex retains its helical structure in chlorinated solvents.

L39 ANSWER 52 OF 53 DISSABS COPYRIGHT (C) 2007 ProQuest Information and Learning Company; All Rights Reserved on STN

ACCESSION NUMBER: 1999:57414 DISSABS Order Number: AAI9932010
TITLE: SELF-ASSEMBLING PEPTIDE NANOTUBES (CYCLIC PEPTIDES)
AUTHOR: HARTGERINK, JEFFREY D. [PH.D.]; GHADIRI, M. REZA [adviser]
CORPORATE SOURCE: THE SCRIPPS RESEARCH INSTITUTE (1179)
SOURCE: Dissertation Abstracts International, (1999) Vol. 60, No. 5B, p. 2134. Order No.: AAI9932010. 152 pages.
DOCUMENT TYPE: Dissertation
FILE SEGMENT: DAI
LANGUAGE: English

AB Self-assembling peptide nanotubes are a new class of supramolecular structures based on the hydrogen bonded stacking of cyclic peptides with an even number of alternating D/L amino acids. This stacking forms an open channel of between 5 and 13A depending on the number of amino acids making up the peptide ring. Because their preparation is based on the self-assembly of relatively small, easily prepared subunits consisting of amino acids, the diameter of the channel formed and the outer surface chemistry of the nanotube can be readily tailored simply by altering the number and choice of amino acids. This flexibility has allowed the preparation of peptide nanotubes with a wide variety of characteristics.

This thesis describes the design, preparation, characterization and functional application of the subset of peptide nanotubes that form well ordered (crystalline) parallel packed arrays. Within this subset of peptide nanotubes two classes, charged and uncharged, are considered. Chapter 1 reviews the work leading up to the preparation of the first self-assembling peptide nanotube in 1993 and the current state of the field. Chapter 2 describes uncharged peptide nanotubes prepared from the cyclic peptides cyclo-[(Gln-D-Xxx)4] (Xxx = Ala, Val, Leu, Phe) by a solvent induced mechanism. Chapter 3 describes three nanotubes prepared from cyclo-[(Xxx-D-Leu) 4] (Xxx = Glu, Lys) by an electrostatic mediated and pH controlled assembly. Finally, chapter 4 discusses results obtained using the outer surface of carboxylate decorated nanotubes as a biomineralization directing agent in the reduction of transition metal salts.

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ACCESSION NUMBER: 1998:162906 SCISEARCH
THE GENUINE ARTICLE: YY786
TITLE: Self-assembly of pyrrole-ferrocene hybrids, determined inter alia by a new chemically induced electrospray mass spectrometry technique
AUTHOR: Scherer M (Reprint); Sessler J L; Moini M; Gebauer A; Lynch V
CORPORATE SOURCE: Univ Texas, Dept Chem & Biochem, Austin, TX 78712 USA (Reprint)
COUNTRY OF AUTHOR: USA
SOURCE: CHEMISTRY-A EUROPEAN JOURNAL, (JAN 1998) Vol. 4, No. 1, pp. 152-158.
ISSN: 0947-6539.
PUBLISHER: WILEY-V C H VERLAG GMBH, PO BOX 10 11 61, D-69451 BERLIN, GERMANY.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 69
ENTRY DATE: Entered STN: 1998
Last Updated on STN: 1998

*ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS*

AB A new approach to organic superstructure self-assembly, based on the use of pyrrole-ester-substituted ferrocenes, is described. Specifically di- and tetrapyrrole-substituted ferrocenes have been prepared. These species are found to form ribbon-like infinite chains in the solid state. In the case of the tetra-substituted system, self-association takes place in solution to produce small but well-defined oligomers. These oligomers were characterized in solution by VPO analysis and in the solution/gas phase by electrospray mass spectrometric methods. In the latter instance the ferrocene moiety was subjected to selective oxidation Frier to analysis, a technique we term oxidative electrospray mass spectrometry (O-ESMS).

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| ☐ | L1 | (peptide or polypeptide ) with amphiphil$ same (nanofiber or nanostructure or nanotube or nanoparticle or nanocluster) | 49 |

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